Tree-like Processor Architecture for Multi-scale, Multi-material and Multi-physics Computation Based on the Material Point Method

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Modeling material response under a high rate of strain requires considerations of the effects of the internal structures of the matter, possibly ranging from the atomistic scale to the mesoscale depending on the strain rate and the material. One of the challenges in the modeling of a multiscale physical problem is to track the change of the internal structures, which often depends on the history of the material deformation in cases of high strain rates [1]. This is because that the time scale for these internal structures to reach an equilibrium state after a rapid deformation is often comparable to the time scale of the deformation. To study dynamic properties of the material, we need to follow the deformation history of the material. In other words, we need a Lagrangian capability in the multiscale method. Many multiscale methods have been mainly focusing on the scale bridging part. These methods have been quite successful in problems involving materials with simple internal structures [2], such as monatomic gas. For complex materials, such as metals with atom lattices in the grains and polymers with molecular chains, the internal structures of the material and their evolutions become important.

In this paper, we propose a multiscale numerical computation scheme that takes the advantages of many multiscale algorithms and is capable of tracking histories of the material. In the method, at a given scale, a physical system is divided into several sub-systems that can be numerically simulated almost independently. These sub-systems only communicate with upper (larger) scale physics. There is no need for direct communication among the sub-systems. In this method, the sub-systems still have needed communications among themselves, but these communications are through their information exchange with the upper scale physics, not directly among the sub-systems. *This numerical property enables us to setup a computer with a tree-like hierarchy of different processors, CPUs and GPUs, with difference computing and communication capabilities.*

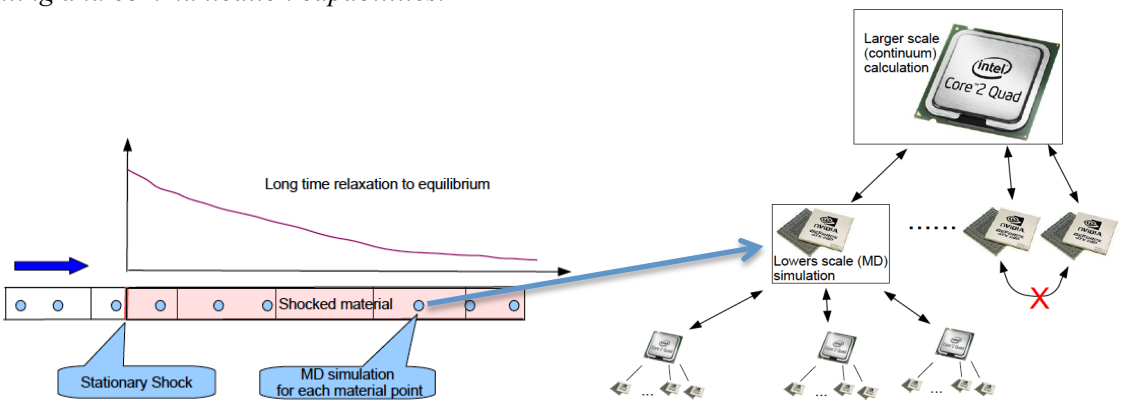

Figure 1. Illustration of one-dimensional shock wave and processor assignment in heterogeneous computer with tree-like processor architecture.

To further explain the proposed idea, we suppose a numerical simulation of a one-dimensional flow with a stationary shock as illustrated in the figure above. For cases of a monatomic gas, one often divides the problem domain into spatially fixed Eulerian cells and takes the advantage of the localized shock front because of the short relaxation time to its thermodynamic equilibrium. The molecular dynamics (MD) simulation is performed only in the cell containing the shock to consider the effects of non-equilibrium thermodynamics. The equation of state for the gas can be used for all other cells. In contrast, for cases of

polymeric liquid, after flowing through the shock front, the time for the material to settle into its thermodynamically equilibrium state could be comparable or longer than the time scale for the material to flow through the tube. In this case, the non-equilibrium thermodynamic effects are important everywhere after the shock. To represent these effects MD simulations need to be performed in all the cells after the shock. To follow the material history, one needs to know from and to which cells the material flows. Therefore, communications among the cells are needed. If each cell is assigned to a processor, communications among processors become necessary.

If the cells used in this problem are Lagrangian cells, then there is no material moving in or out of a cell, and the direct communications between cells, or processors assigned to calculate the cells become unnecessary. With the lower scale physics simulated using MD simulations at each cell, the statistical method [3,4] can used to calculate the higher-level physical quantities, such as the pressure and temperature. The pressures calculated in these cells are then used to calculate the pressure gradient across the cells and then used to accelerate the material and to find the new velocity. The cell-to-cell communication happens at the larger scale (continuum) level. With the update velocity field, we can calculate the updated volumetric deformation rate. This updated volumetric deformation rate is then communicated to the Lagrangian cells to further the MD simulation. All cell-to-cell communication is through larger scale physics calculation; no direct cell-to-cell communication is needed in this MD simulation using Lagrangian cells moving with the material. This is the advantage of a Lagrangian method in the computation of multiscale physics. However, this advantage disappears in two- or three-dimensional problems with large material deformation because of the distortion of the Lagrangian cells.

To take the advantage of the Lagrangian method and to avoid the cell distortion difficulty, we use the material point method (MPM), especially the recently improved version of the method, the dual domain material point (DDMP) method [5,6]. In the method, we use Lagrangian material points to follow the deformation history of the material and use Eulerian cells to calculate the gradients at the continuum scale. The MPM is the advanced version of particle in cell method and is similar to the finite element method based on the weak solution theory to partial differential equations [7]. The original MPM suffers numerical stability issues when applied to problems with large deformations. This issue is resolved in the DDMP method. The method has been applied to many problems with high rate of strain and large deformations, such as projectile impact, hypervelocity pulverization, and fluid-structure interactions from the meso to macroscopic scales, with heat transfer, species diffusion and chemical reactions in both ductile and brittle materials. In all these examples, the computations of the material or chemical reaction models are performed on the material points without direct communication with other material points.

Instead of using material and chemical reaction models to calculate the model quantities, for non-equilibrium thermodynamic problems, MD simulations can be performed to calculate them on material points [8]. A processor can be dedicated to a material point. Furthermore, if a material point represents a large piece of a material with further internal structures, such as a group of metal grains with different crystal orientations, we can assign a cluster of processors to the material point. Within the cluster, the material point method can be used to consider anisotropic elasticity, plasticity and voids of the crystals, while atomistic simulation is performed to study effects of dislocations and grain boundaries running on lower level processors.

In this proposed approach, the load balancing among the same level of processors can be easily achieved. The load balance and power consumption of different levels of processors need to be optimized. We also need to study the consistence between the results obtained from the MD simulation performed over the entire problem domain as one problem and the results from this proposed multiscale approach with the MD simulations performed on material points as sub-systems. In more complex systems, such as fluid-structure or multi-material interactions, it could be necessary to construct branches of the processor tree for materials with different speed ratios among the different levels of processors because of the physics in the materials.

References:

1. Zhang, D. Z., Liu, C., & Harlow, F. H. 2002, Effects of non-uniform segment deformation on the constitutive relations of polymeric solids. *Phys. Rev. E*. **66**, 051806.
2. E, w., & Huang, Z., Matching Condition in Atomistic-Continuum modeling of materials, *Phys. Rev. Letts.* **87**, 135501
3. Zhang, D. Z., Ma, X. & Rauenzahn, R.M. 2006, Inter-species stress in momentum equations for dense binary particulate systems. *Phys. Rev. Letts.*, **97**, 048301.
4. Zhang, D. Z., VanderHeyden, W.B., Zou, Q. & Padial-Collins, N. T. 2007, Pressure calculation in disperse and continuous multiphase flows. *Int. J. Multiphase Flow*. **33**, pp. 86-100.
5. Zhang, D. Z., Ma X. & Giguere, P.T., 2011, Material point method enhanced by modified gradient of shape function, *J. comp. phys.* **230**, pp 6379–6398.
6. Ma, X., Zhang, D.Z., Giguere, P. T. & Liu, C., 2013, Axisymmetric computation of Taylor cylinder impacts of ductile and brittle materials using original and dual domain material point methods, *Int. J. Impact Engrg.* **54**, pp 96-104.
7. Sulsky, D. Chen, Z. and Schreyer, H.L, 1994, A particle method for history-dependent materials, *Comput. Methods Appl. Mech. Engrg.* **118**, pp 179-196.
8. Mao, S., Ma, X., DuPont, V. & Zhang, D.Z., 2012, Scale-bridging schemes based on the material point method. APS/DFD meeting, Nov. 18-20. San Diego, CA.